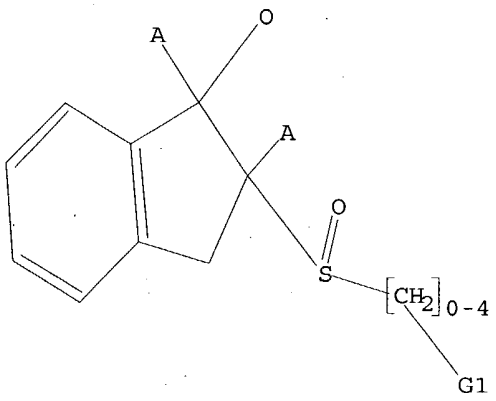
L4 STRUCTURE UPLOADED

=> que L4

L5 QUE L4

=> d
L5 HAS NO ANSWERS
L4 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.
L5 QUE ABB=ON PLU=ON L4

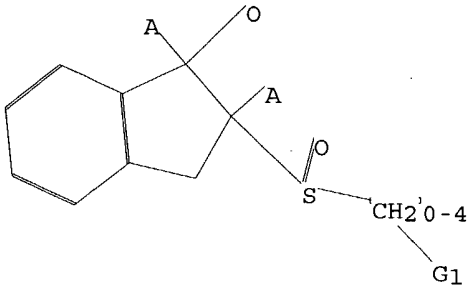
=> s l5 full
FULL SEARCH INITIATED 16:30:51 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED - 4755 TO ITERATE

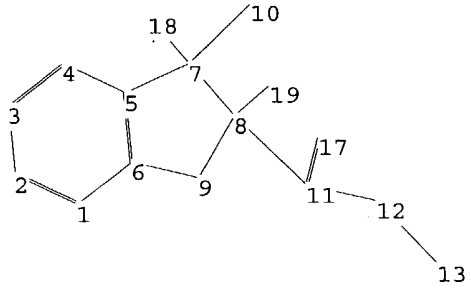
100.0% PROCESSED 4755 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.07

L6 0 SEA SSS FUL L4

=>

=>
Uploading C:\Program Files\Stnexp\Queries\10692735.str





chain nodes :
10 11 12 13 17 18 19
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-10 7-18 8-11 8-19 11-12 11-17 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-10 7-18 8-9 8-11 8-19 11-17 12-13
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:Cy,Ak

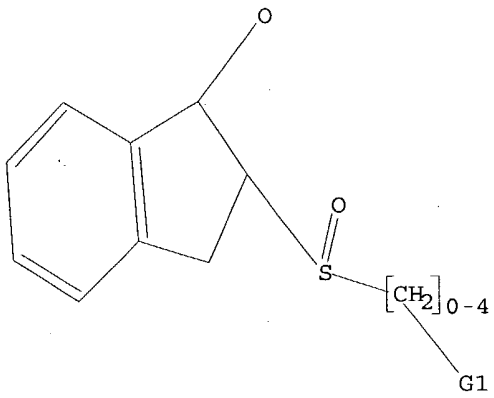
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 17:CLASS 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d
L2 HAS NO ANSWERS
L1 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PLU=ON L1

=> s l2
SAMPLE SEARCH INITIATED 14:37:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 721 TO ITERATE

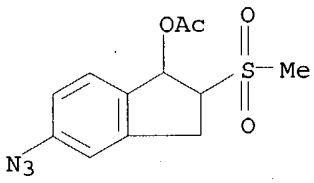
100.0% PROCESSED 721 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 12810 TO 16030
PROJECTED ANSWERS: 4 TO 200

L3 4 SEA SSS SAM L1

=> d scan

L3 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 5-azido-2,3-dihydro-2-(methylsulfonyl)-, acetate (ester) (9CI)
MF C12 H13 N3 O4 S



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l2 full
FULL SEARCH INITIATED 14:37:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 14788 TO ITERATE

100.0% PROCESSED 14788 ITERATIONS 69 ANSWERS
SEARCH TIME: 00.00.01

L4 69 SEA SSS FUL L1

=>

=>

=> s l4 and sulfox?
  9366 SULFOX?
L5 0 L4 AND SULFOX?

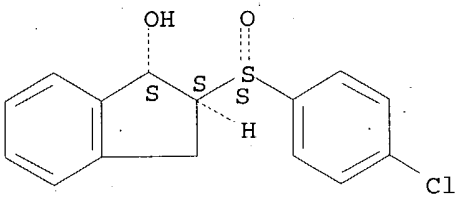
=> s l4 and sulfo?
  1667899 SULFO?
L6 39 L4 AND SULFO?

=> s l4 not l6
L7 30 L4 NOT L6

=> d scan

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2β(R*)]- (9CI)
MF C15 H13 Cl O2 S

Relative stereochemistry.

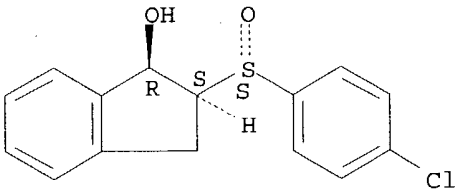


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2α(S*)]- (9CI)
MF C15 H13 Cl O2 S

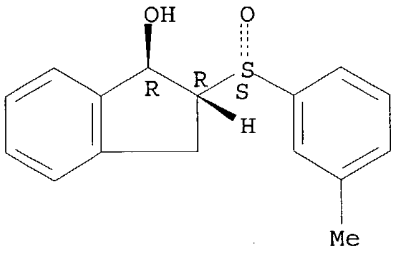
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α,2β(S*)]- (9CI)
MF C16 H16 O2 S

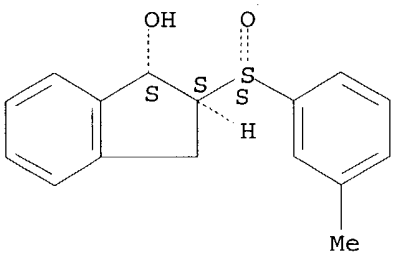
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α,2β(R*)]- (9CI)
MF C16 H16 O2 S

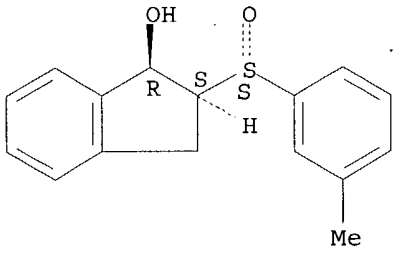
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α,2α(S*)]- (9CI)
MF C16 H16 O2 S

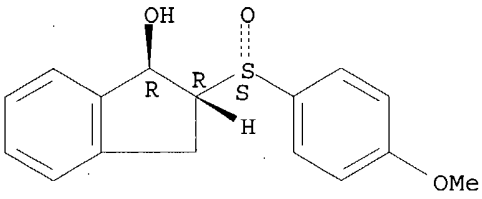
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2β(S*)]- (9CI)
MF C16 H16 O3 S

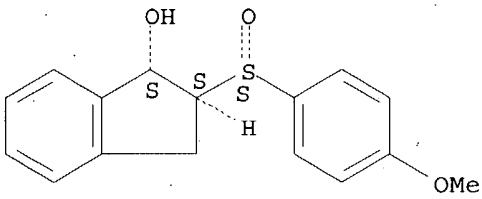
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2β(R*)]- (9CI)
MF C16 H16 O3 S

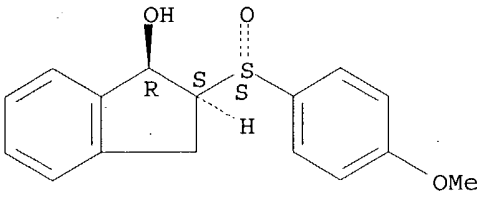
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

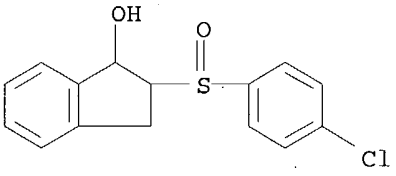
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2α(S*)]- (9CI)
MF C16 H16 O3 S

Relative stereochemistry.



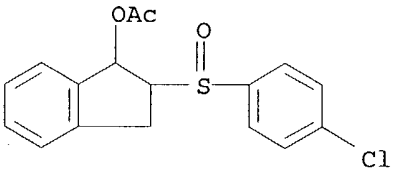
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI)
MF C15 H13 Cl O2 S



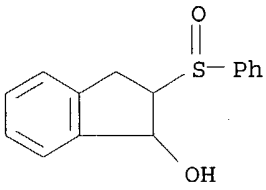
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, acetate (9CI)
MF C17 H15 Cl O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

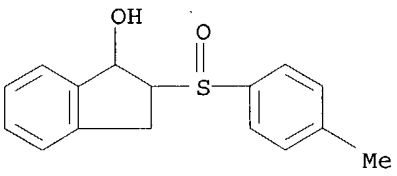
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI)
MF C15 H14 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

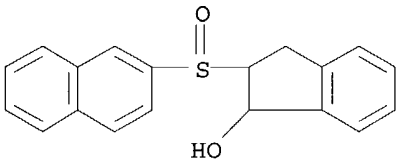
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI)
MF C16 H16 O2 S



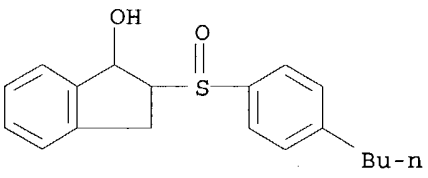
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI)
MF C19 H16 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

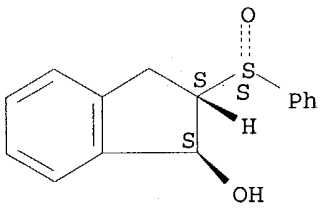
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Indanol, 2-[(p-butylphenyl)sulfinyl]- (7CI)
MF C19 H22 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

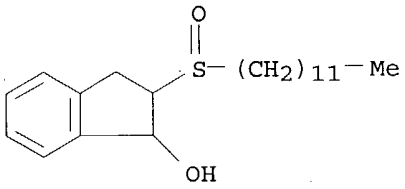
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI)
MF C15 H14 O2 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

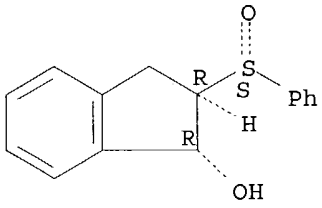
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Indanol, 2-(dodecylsulfinyl)- (6CI)
MF C21 H34 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2S)-rel- (9CI)
MF C15 H14 O2 S

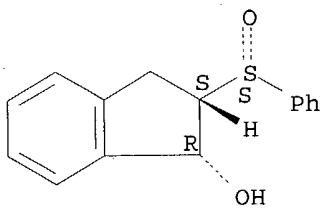
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2R)-rel- (9CI)
MF C15 H14 O2 S

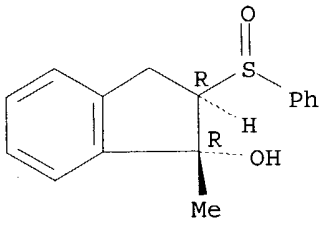
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-,
    (1α,2β)- (9CI)
MF C16 H16 O2 S

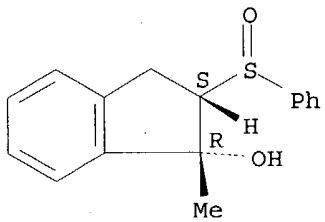
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

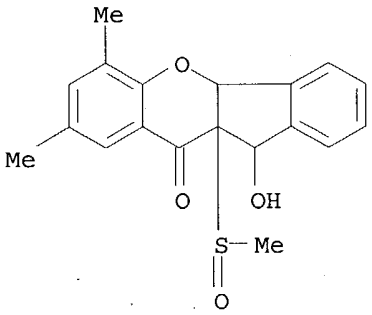
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-,
    (1α,2α)- (9CI)
MF C16 H16 O2 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benz[b]indeno[2,1-e]pyran-10(4bH)-one, 10a,11-dihydro-11-hydroxy-6,8-dimethyl-10a-(methylsulfinyl)- (9CI)
MF C19 H18 O4 S

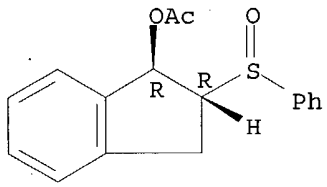


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2R)-rel- (9CI)
MF C17 H16 O3 S

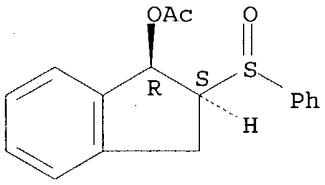
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

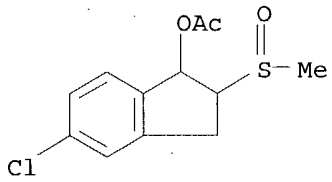
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2S)-rel- (9CI)
MF C17 H16 O3 S

Relative stereochemistry.



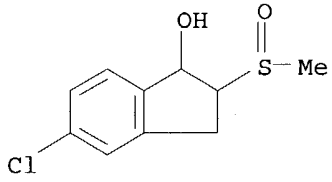
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)-, acetate (9CI)
MF C12 H13 Cl O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

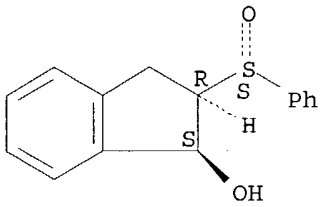
L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)- (9CI)
MF C10 H11 Cl O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1S-[1α,2α(R*)]]- (9CI)
MF C15 H14 O2 S

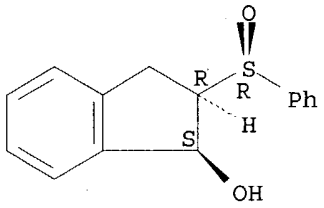
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1S-[1α,2α(S*)]]- (9CI)
MF C15 H14 O2 S

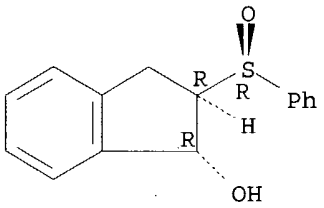
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(R*)]]- (9CI)
MF C15 H14 O2 S

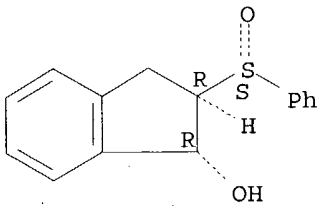
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(S*)]]- (9CI)
MF C15 H14 O2 S

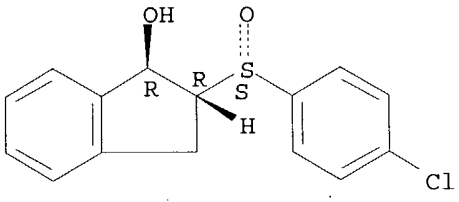
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2β(S*)]- (9CI)
MF C15 H13 Cl O2 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	165.12	165.96

FILE 'CAPLUS' ENTERED AT 14:39:01 ON 28 APR 2004
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FILE COVERS 1907 - 28 Apr 2004 VOL 140 ISS 18
FILE LAST UPDATED: 27 Apr 2004 (20040427/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

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=> s l7
L8          22 L7

=> d ibib abs hitstr 1-22

L8   ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:202618  CAPLUS
DOCUMENT NUMBER:          138:221365
TITLE:                    Preparation of indan-1-ols as appetite depressants
INVENTOR(S):              Jaehne, Gerhard; Krone, Volker; Bickel, Martin;
                          Gossel, Matthias
PATENT ASSIGNEE(S):       Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE:                   PCT Int. Appl., 53 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2003020696      A1   20030313       WO 2002-EP9206   20020817
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
     DE 10142667        A1   20030327       DE 2001-10142667 20010831
     US 2003114681      A1   20030619       US 2002-231394   20020830
     US 6657086         B2   20031202
     US 2004068016      A1   20040408       US 2003-665021   20030922
PRIORITY APPLN. INFO.:                   DE 2001-10142667 A  20010831
                                         US 2002-231394   A3 20020830
OTHER SOURCE(S):          MARPAT 138:221365
GI
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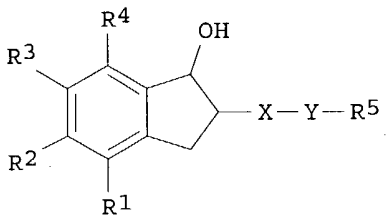

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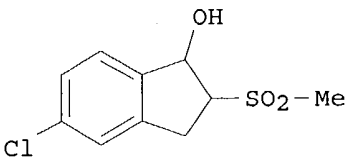


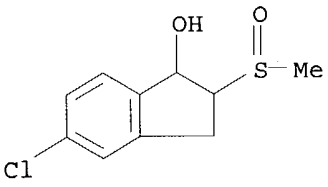
II

AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; X = S, SO, SO2; Y = (CH2)p; p = 0-3; R5 = CF3, alkyl, cycloalkyl] and their pharmaceutically acceptable salts were prepared For example, NaBH4 mediated reduction of 5-chloro-2-methylsulfonylindan-1-one, e.g., prepared from 2-bromo-5-chloroindan-1-one in 2-steps, provided indanol II. In milk

consumption studies with female NMRI mice, indanol II exhibited very good anorectic effects, i.e., 50% decrease in milk consumption verses control.

IT **500910-96-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indanols as appetite depressants)

RN 500910-96-3 CAPLUS
CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)- (9CI) (CA INDEX NAME)

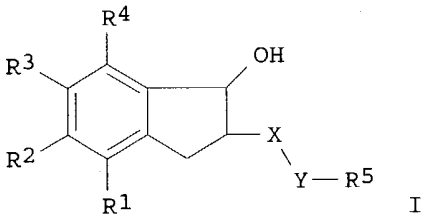


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:202465 CAPLUS
DOCUMENT NUMBER: 138:221361
TITLE: Preparation of indan-1-ols for producing drugs for the prophylaxis or treatment of obesity
INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin; Gossel, Matthias
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020263	A1	20030313	WO 2002-EP9205	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142666	A1	20030320	DE 2001-10142666	20010831
US 2003134879	A1	20030717	US 2002-231183	20020830

PRIORITY APPLN. INFO.: DE 2001-10142666 A 20010831
OTHER SOURCE(S): MARPAT 138:221361
GI



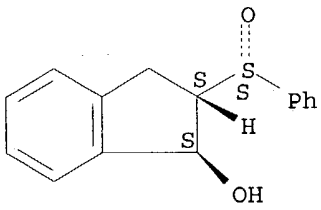
I

AB Title compds. [I; R1-R4 = H, F, Cl, Br, I, cyano, N3, NO2, OH, alkoxy, cycloalkoxy, benzyloxy, phenoxy, alkylcarbonyloxy, etc.; X = S, SO, SO2; Y = (CH2)p; p = 0-3; R5 = CF3, (fluorinated) alkyl, cycloalkyl, etc.], were prepd for producing a drug for body weight loss of mammals. Thus, 5-chloro-2-methylsulfonylindan-1-one (preparation given) and NaBH4 in EtOH were put into a ultrasound bath for 4 h followed by stirring with 2N HCl to give 5-chloro-2-methylsulfonylindan-1-ol. The latter at 20 mg/kg i.p. was applied in female NMRI mice and gave 50% reduction of milk consumption of the treated mice.

IT **95720-00-6P 134779-81-0P 134779-82-1P 500910-96-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indanols for producing drugs for prophylaxis or treatment of obesity)

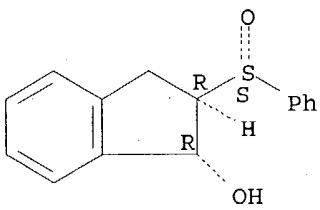
RN 95720-00-6 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



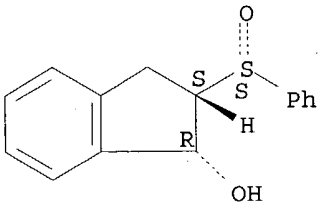
RN 134779-81-0 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

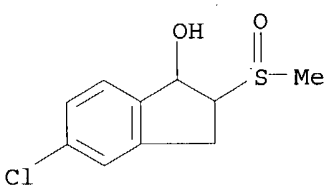


RN 134779-82-1 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 500910-96-3 CAPLUS
CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)- (9CI) (CA INDEX NAME)

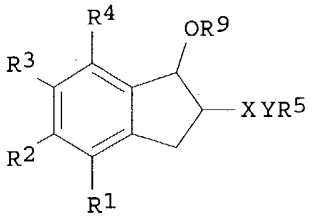


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:202409 CAPLUS
DOCUMENT NUMBER: 138:226750
TITLE: Use of C2-substituted indan-1-ol derivatives in antiobesity drugs
INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin; Gossel, Matthias
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020199	A1	20030313	WO 2002-EP9199	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142660	A1	20030320	DE 2001-10142660	20010831
US 2003134881	A1	20030717	US 2002-230379	20020829
US 6667345	B2	20031223		

PRIORITY APPLN. INFO.: DE 2001-10142660 A 20010831
OTHER SOURCE(S): MARPAT 138:226750
GI



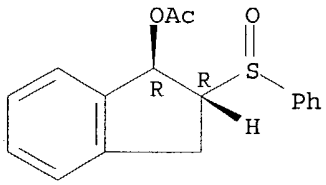
I

AB The invention relates to the use of C2-substituted indan-1-ol systems, and to the physiol. tolerable salts and the physiol. functional derivs. of the same, for producing medicaments used to reduce the weight of mammals, and for the prophylaxis or the treatment of obesity. The invention also relates to the use of compds. of formula (I), wherein the radicals have the cited designations, and to the physiol. tolerable salts and the physiol. functional derivs. of the same, for producing a medicament for the prophylaxis or the treatment of obesity. The antiobesity drugs can be combined with other active ingredients, e.g. cathine, phenylpropanolamine, amfepramone, mefenorex. Capsules, tablets, emulsions, dragees and suppositories are prepared containing the indan-1-ol derivative antiobesity drugs.

IT **500770-90-1 500770-91-2 500770-94-5**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of C2-substituted indan-1-ol derivs. in antiobesity drugs)

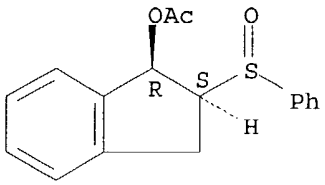
RN 500770-90-1 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

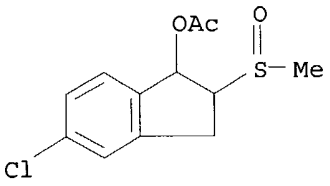


RN 500770-91-2 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 500770-94-5 CAPLUS
CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)-, acetate (9CI) (CA INDEX NAME)

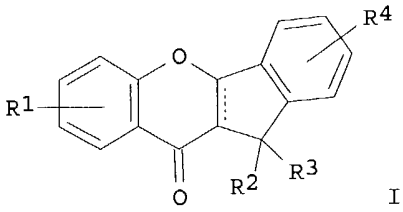


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:733853 CAPLUS
DOCUMENT NUMBER: 131:322537
TITLE: Preparation of 10,11-dihydro-11-hydroxybenz[b]indeno[2,1-e]pyran-10-ones and analogs for enhancing biosynthesis of erythropoietin
INVENTOR(S): Williams, Jonathan Gareth; Houck, David R.; Smith, David Edward; Rathbone, Daniel Lee; Billington, David Charles; Golding, Bernard T.; Collington, Eric W.; Kitchin, John; Rich, Nicholas
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: U.S., 13 pp., Cont.-in-part of U.S. 5,882,436.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5985913	A	19991116	US 1998-69693	19980429

PRIORITY APPLN. INFO.: US 1996-32268P P 19961129
US 1997-978346 A2 19971126
OTHER SOURCE(S): MARPAT 131:322537
GI



I

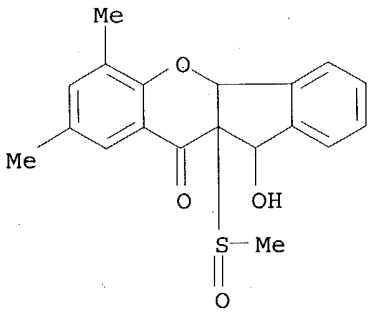
AB Title compds. [I; R1,R4 = H or 1-4 of halo, alkyl, alkoxy, etc.; R2 = OR10 and R3 = H or R2R3 = O; R10 = H or alkanoyl; dashed line = optional addnl. bond] were prepared Thus, 3',5'-dimethyl-2'-hydroxy-2-methylsulfinylacetophenone (preparation given) was cyclocndensed with 2-(OHC)C6H4CHO to give I (R1 = 6,8-Me2, R2 = OH, R3 = R4 = H, dashed line = bond). Data for biol. activity of I were given.

IT **249514-81-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 10,11-dihydro-11-hydroxybenz[b]indeno[2,1-e]pyran-10-ones

and analogs for enhancing biosynthesis of erythropoietin)

RN 249514-81-6 CAPLUS

CN Benz[b]indeno[2,1-e]pyran-10(4bH)-one, 10a,11-dihydro-11-hydroxy-6,8-dimethyl-10a-(methylsulfinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:409577 CAPLUS

DOCUMENT NUMBER: 121:9577

TITLE: Reactions of η2-(2-acylaryl-C,O)tetracarbonylmanganese(I) complexes with some vinyl sulfur compounds

AUTHOR(S): Cambie, Richard C.; Rutledge, Peter S.; Welch, David R.; Woodgate, Paul D.

CORPORATE SOURCE: Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, N. Z.

SOURCE: Journal of Organometallic Chemistry (1994), 467(2), 237-44
CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:9577

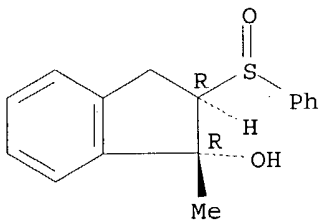
AB The thermally promoted reactions of some Ph and diterpenoid η2-(2-acylaryl-C,O)tetracarbonylmanganese(I) complexes with Ph vinyl sulfone, Me vinyl sulfone, or Ph vinyl sulfoxide, have been investigated. The major products from the diterpenoid complexes arises from insertion followed by reductive demetalation; cyclopenta-annulation, when it occurs, is a minor process. Liberation of the metal-free adducts from their Mn-containing precursors requires treatment with either acid or photolysis-oxidation

IT **155519-28-1P 155519-29-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 155519-28-1 CAPLUS

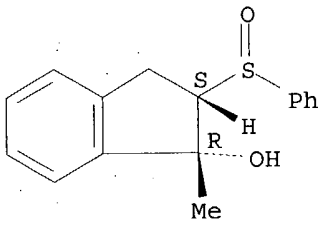
CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-, (1α,2β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155519-29-2 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-, (1α,2α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



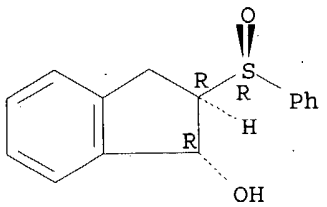
L8 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:558285 CAPLUS
DOCUMENT NUMBER: 115:158285
TITLE: Cooxidation reaction of indene and aromatic thiols in the presence of ovalbumin
AUTHOR(S): Freer, Juanita; Fuentealba, Cecilia; Gonzalez, Elizabeth; Baeza, Jaime
CORPORATE SOURCE: Dep. Quim., Univ. Concepcion, Concepcion, Chile
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1991), 61(1-2), 41-8
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:158285

AB The thiol olefin cooxidn. reaction (TOCO) between indene and aromatic thiols in presence of ovalbumin has been studied in hexane. While this reaction under normal conditions leads to the formation of 6 products, in the presence of OVA give stereospecifically only the trans-2-phenylmercapto-1-indanol derivative on the protein surface.

IT **32819-87-7P 32819-88-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

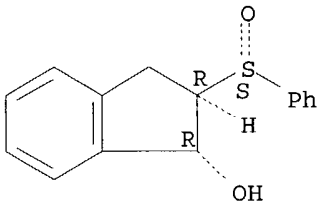
RN 32819-87-7 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 32819-88-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(S*)]]- (9CI) (CA INDEX NAME)

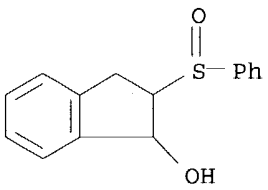
Absolute stereochemistry.



L8 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:539316 CAPLUS
DOCUMENT NUMBER: 115:139316
TITLE: Fuel instability model studies: the liquid-phase cooxidation of thiols and indene by oxygen
AUTHOR(S): Morris, Robert E.; Mushrush, George W.
CORPORATE SOURCE: Nav. Technol. Cent. Saf. Survivabil., Nav. Res. Lab., Washington, DC, 20375, USA
SOURCE: Energy & Fuels (1991), 5(5), 744-8
CODEN: ENFUEM; ISSN: 0887-0624
DOCUMENT TYPE: Journal
LANGUAGE: English

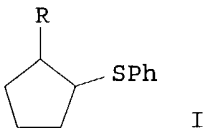
AB Instability problems in middle distillate fuels were correlated with the presence of both active olefin species and heteroat. compds. such as thiols. The type of S compound rather than the total S concentration is the key to fuel instability reactions. Low concns. of thiols will act as radical traps to inhibit autoxidn. When added to a fuel, thiols accelerated the rate of Oxidation without a commensurate increase in peroxidn. Evidence for the oxidative addition of thiols to olefins was observed by studying the addition of thiophenol to indene in a model fuel during stressing in both a model system at 100-120° and in the jet fuel thermal oxidation test apparatus at 350°. Similarities and differences were found in the 2 systems, with the product distribution being temperature dependent. This could account, in part, for the differences in thiol influences on autoxidn. observed in model systems and in fuels.

IT **92621-28-8P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of indene with thiophenol and oxygen, jet fuel instability model study in relation to)
RN 92621-28-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:448966 CAPLUS
DOCUMENT NUMBER: 115:48966
TITLE: Cooxidation between thiophenol and cyclopentene
AUTHOR(S): Freer, Juanita; Palma, Graciela; Fuentealba, Cecilia; Pena, Monica; Baeza, Jaime
CORPORATE SOURCE: Dep. Quim., Univ. Concepcion, Concepcion, Chile

SOURCE: Boletin de la Sociedad Chilena de Quimica (1991), 36(1), 11-16
CODEN: BOCQAX; ISSN: 0366-1644
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI



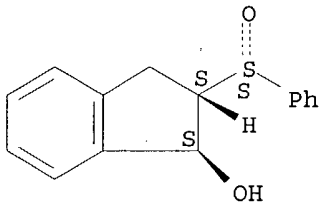
I

AB Treatment of thiophenol with cyclopentene in the presence of O2 gene adduct I (R = H) as well as cooxidn. products, i.e., cis- and trans-I (R = OH) and the sulfoxide derivs. The reaction of thiophenol with indene gave similar results.

IT **95720-00-6P 134779-81-0P 134779-82-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

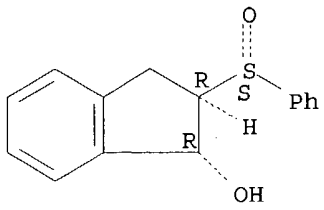
RN 95720-00-6 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



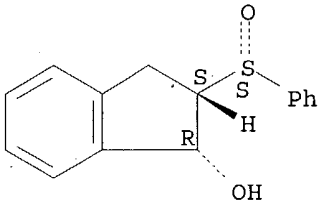
RN 134779-81-0 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 134779-82-1 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

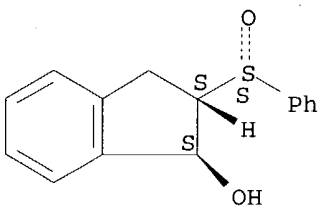


L8 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:224013 CAPLUS
DOCUMENT NUMBER: 108:224013
TITLE: Liquid-phase oxidation of thiophenol and indene by tert-butyl hydroperoxide and oxygen
AUTHOR(S): Mushruch, George W.; Watkins, John M.; Hazlett, Robert N.; Hardy, Dennis R.; Eaton, Harold G.
CORPORATE SOURCE: Nav. Res. Lab. Code 6180, Washington, DC, 20375-5000, USA
SOURCE: Fuel Science & Technology International (1988), 6(2), 165-83
CODEN: FSCTEG; ISSN: 0884-3759
DOCUMENT TYPE: Journal
LANGUAGE: English

AB tert-Bu hydroperoxide (I) or O initiated the oxidation of thiophenol in the presence of indene was examined in C6H6 at 120°. The reaction is kinetically complex, but it was possible to relate the product distribution to a few competing reactions. The product mixture was determined for several reaction time periods. The product slate was similar for all time periods, but yields of the individual components varied significantly with increasing reaction time. Gaseous products included isobutylene and a trace of CH4. The major product from I was tert-BuOH. The major product observed from thiophenol was Ph2S2. Addition products included the major product 2-phenylthiyl indan. Oxidation products included indanols, indanones, and the sulfoxide and sulfone of the major product 2-phenylthiyl indan. Solvent participation was noted by trace amts. of toluene.

IT **95720-00-6P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in indene reaction with thiophenol and oxygen or tert-Bu hydroperoxide, jet fuel in relation to)
RN 95720-00-6 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L8 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:148840 CAPLUS
DOCUMENT NUMBER: 102:148840
TITLE: Stereoselective oxidative addition of benzenethiol to indene in the presence of ovalbumin

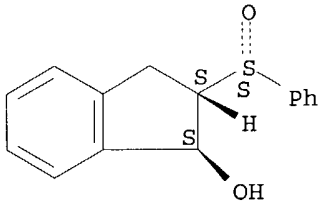
AUTHOR(S): Baeza, Jaime; Freer, Juanita; Palma, Graciela
CORPORATE SOURCE: Dep. Quim., Univ. Concepcion, Concepcion, Chile
SOURCE: Monatshefte fuer Chemie (1984), 115(11), 1369-71
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:148840

AB The oxidative addition of PhSH to indene in the presence of ovalbumin produces only trans-anti-2-phenylsulfinyl-1-indanol. This reaction may be considered as a biomimetic model of detoxification of certain hydrocarbons by the liver.

IT **95720-00-6**
RL: PROC (Process)
(stereospecific formation of, in presence of ovalbumin)

RN 95720-00-6 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

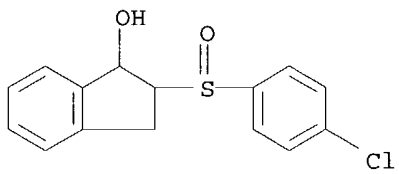


L8 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:190435 CAPLUS
DOCUMENT NUMBER: 88:190435
TITLE: Thiol-olefin cooxidation reaction. 6. A new convenient route to 1-substituted indenes. Indenone as dienophile in Diels-Alder reactions
AUTHOR(S): Szmant, H. Harry; Nanjundiah, Raghunath
CORPORATE SOURCE: Dep. Chem. Chem. Eng., Univ. Detroit, Detroit, MI, USA
SOURCE: Journal of Organic Chemistry (1978), 43(9), 1835-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:190435

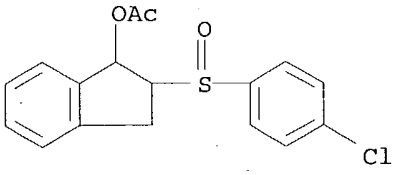
AB 2-(4-Chlorophenylsulfinyl)-1-indanone was decomposed in refluxing toluene to give indenone which was trapped by cyclopentadiene, hexachlorocyclopentadiene, and anthracene to give the resp. Diels-Alder adducts.

IT **62967-56-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, 1-indanone analog from)

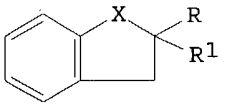
RN 62967-56-0 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



IT **65495-98-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65495-98-9 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, acetate (9CI) (CA INDEX NAME)



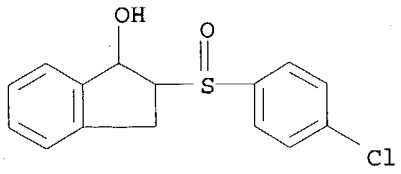
L8 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:422824 CAPLUS
DOCUMENT NUMBER: 87:22824
TITLE: A new route to 1,2-indanedione
AUTHOR(S): Szmant, H. Harry; Nanjundiah, Raghunath
CORPORATE SOURCE: Dep. Chem. Chem. Eng., Univ. Detroit, Detroit, MI, USA
SOURCE: Organic Preparations and Procedures International (1977), 9(1), 35-8
CODEN: OPPIAK; ISSN: 0030-4948
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:22824
GI



I

AB O was bubbled through a mixture of indene and p-ClC6H4SH in isooctane at room temperature and the resultant mixture of isomeric indanol sulfoxides (I; X = CHOH; R = H; R1 = p-ClC6H4SO) was oxidized with Jones reagent to give indanone sulfoxide (I; X = CO; R and R1 as before), which was refluxed with MeOH in the presence of iodine and the product (I; X = CO; R = R1 = OMe) was deketalized with EtOH-H2SO4 at reflux to give 1,2-indandione [I; X = CO; (RR1) = O].

IT **62967-56-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Jones oxidation of)
RN 62967-56-0 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



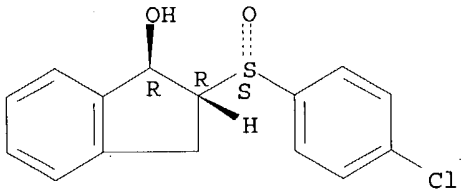
L8 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:170438 CAPLUS
DOCUMENT NUMBER: 86:170438
TITLE: The thiol-olefin cooxidation (TOCO) reaction. IV. Temperature effects on product distribution in the TOCO reaction of indene and aromatic thiols
AUTHOR(S): Szmant, H. H.; Mata, A. J.; Namis, A. J.; Panthananickal, A. M.
CORPORATE SOURCE: Dep. Chem., Univ. Detroit, Detroit, MI, USA
SOURCE: Tetrahedron (1976), 32(22), 2665-80
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stereochem. of the TOCO reaction of indene with RC6H4SH (R = 4-Cl, 4-MeO, 3-Me) is temperature dependent. Increasing amts. of cis addition products are formed as the temperature is lowered to -23° and raised to .apprx.60°. The sensitivity of the temperature effect depends on the electronic character of the substituent in RC6H4SH. The effect of solvent, addition of cumyl hydroperoxide, K2S2O8, galvinoxyl, PhNOCMe3, Na2S2O3, and Na tetrathionate, and the kinetics of the TOCO reaction were determined

IT **62703-00-8P 62703-01-9P 62703-02-0P**
62703-05-3P 62703-06-4P 62703-07-5P
62703-10-0P 62703-11-1P 62703-12-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

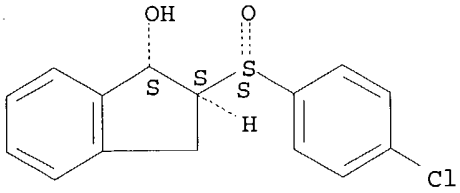
RN 62703-00-8 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2β(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



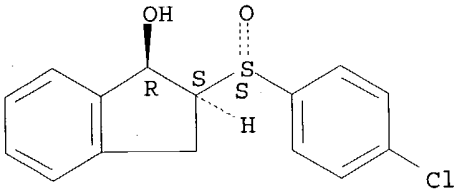
RN 62703-01-9 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2β(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



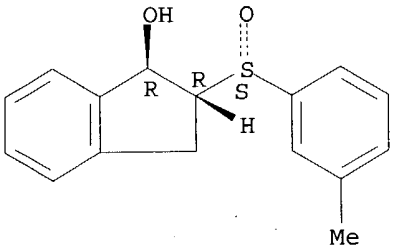
RN 62703-02-0 CAPLUS
CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α,2α(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



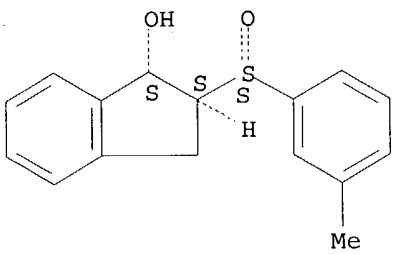
RN 62703-05-3 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α,2β(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 62703-06-4 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α,2β(R*)]- (9CI) (CA INDEX NAME)

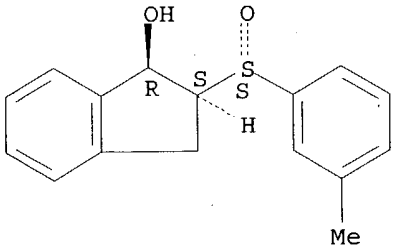
Relative stereochemistry.



RN 62703-07-5 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-,

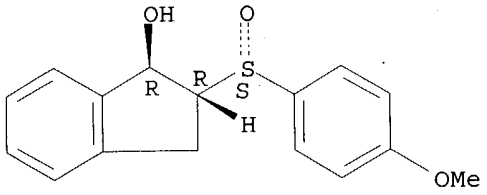
[1α,2α(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



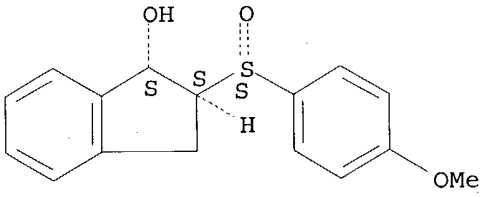
RN 62703-10-0 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2β(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



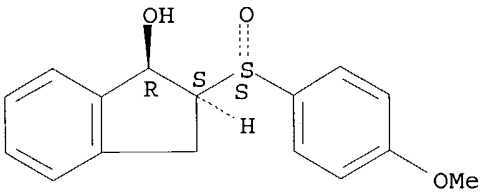
RN 62703-11-1 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2β(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 62703-12-2 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1α,2α(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



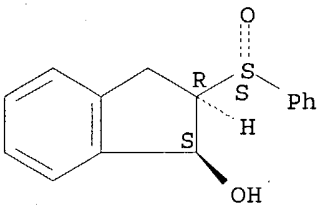
L8 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:85045 CAPLUS
DOCUMENT NUMBER: 76:85045
TITLE: Nonstereospecific oxidative addition of benzenethiol to indene
AUTHOR(S): Szmant, H. Harry; Rigau, Juan J.
CORPORATE SOURCE: Puerto Rico Nucl. Cent., Univ. Puerto Rico, San Juan, P. R.
SOURCE: Journal of Organic Chemistry (1972), 37(3), 447-51
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The oxidative addition of benzenethiol to indene produces a mixture of three isomeric 2-phenylsulfinylindanols that contains 14-18% of the cis-hydroxy sulfoxide contrary to previous claims that this reaction leads stereospecifically only to trans addition products. The fourth isomeric 2-phenylsulfinylindanol (cis-syn) was prepared by the oxidation of the sulfide precursor. Examination of the concentration dependence of H bonding, of the NMR spectra, and of the relative yields permits assignment of the configurations at the S atom in all isomers.

IT **32785-03-8P 32819-85-5P 32819-87-7P 32819-88-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

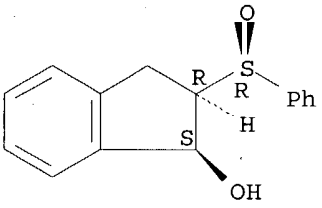
RN 32785-03-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1S-[1α,2α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



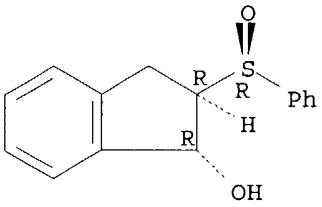
RN 32819-85-5 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1S-[1α,2α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



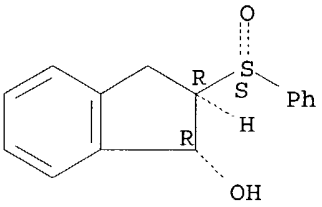
RN 32819-87-7 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 32819-88-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-[1α,2β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:475774 CAPLUS
DOCUMENT NUMBER: 57:75774
ORIGINAL REFERENCE NO.: 57:15030e-i
TITLE: Hydroperoxides and sulfoxides
INVENTOR(S): Oswald, Alexis A.; Rupar, Charles B.; Greenwood, Sydney H.J.
PATENT ASSIGNEE(S): Esso Research and Engineering Co.
SOURCE: 8 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3043824		19620710	US	19590928

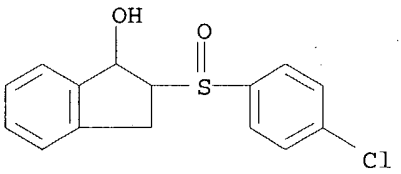
AB Co-oxidation of RSH with olefins or diolefins in the presence of O at 0° produced new sulfoxides and hydroperoxides. Ultraviolet light and hydroperoxides were found to be effective catalysts for the oxidation Thus, 20.2 g. n-C12H25SH and 10.4 g. styrene were dissolved in 150 cc. n-C7H16 in 500 cc. quartz bottle and irradiated with ultraviolet light (or hydroperoxides added). Air was passed through the solution via sintered glass and filtered after 0.5 hr. to give 18.7% 2-phenyl-2-hydroperoxyethyl n-dodecyl sulfide. Similarly prepared were 1-hydroperoxy-4-phenylthio-2-butene, 1-hydroperoxy-4-(2- naphthylthio)-2-pentene, 2-hydroperoxy-4-(2-naphthylthio)-2cyclopentene, and 4,7-methylene-5-(2-naphthylthio)-6-hydroperoxy-4,5,6,7,8,9-hexahydroindene. The filtrate was treated with air 6 hrs. and filtered to give 9 g. 2-phenyl-2hydroxyethyl n-dodecyl sulfoxide (I), m. 107-9° (benzene-nheptane). The filtrate gave a mixture of isomeric I, m. 66-9°. Similarly prepared were the following sulfoxides, where R1 = C16H33CH(OH)CH2, R2 = p-MeC6H4, R3 = naphthyl, R4 = p-ClC6H4, R5 = PhCH(OH)CH2, R6 = PhCMe(OH)CH2, R7 = C12H25, and R8 = 2-(1-hydroxyindanyl): PhSOCH2CH(OH)C10H21, m. 67-8°; PhSOR1, m. 51-2°; R2SOR1, m. 60-2°; R3SOR1, m. 88-90°; R4SOR1, m. 65-6.5°; R5SOPh, m. 123-30°; R5SOR3, m. 145-7°; R5SOR4, m. 156.5-8.5°; R6SOR3, m. 114-18°; R6SOR7, m. 47.5-8.5°; R8SOPh, m. 158-9° (decomposition); R8SOR2,

166-7.5° (decomposition); R8SOR4 m. 144-6°; R8SOR3, m. 149-50°; and R8SOR7, m. 107-9°. The hydroxy sulfoxide products of dicyclopentadiene-RSH co-oxidns. were useful as petroleum additives, antistatic agents, and pesticides. The OH group may be esterified with H2SO4 and converted to detergents. The hydroperoxides are useful as radical polymerization promoters and can be alkylated to give surfactive agents. Co-oxidation can be utilized to remove dienes from steam-cracked naphtha and for removal of RSH from petroleum.

IT **62967-56-0**, 1-Indanol, 2-[(p-chlorophenyl)sulfinyl]-
92621-28-8, 1-Indanol, 2-(phenylsulfinyl)- **93434-18-5**,
1-Indanol, 2-(p-tolylsulfinyl)- **94305-49-4**, 1-Indanol,
2-(2-naphthylsulfinyl)- **102456-32-6**, 1-Indanol,
2-(dodecylsulfinyl)-
(preparation of)

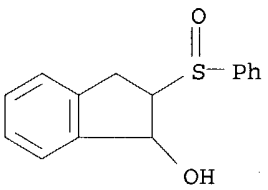
RN 62967-56-0 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



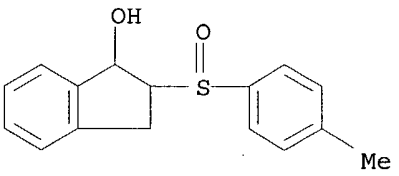
RN 92621-28-8 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



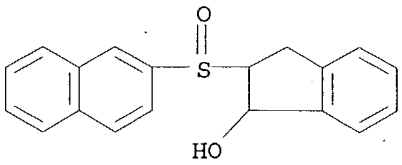
RN 93434-18-5 CAPLUS

CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)

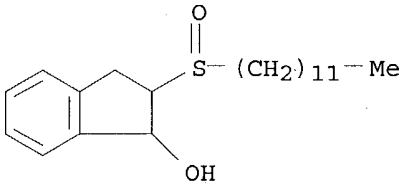


RN 94305-49-4 CAPLUS

CN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



RN 102456-32-6 CAPLUS
CN 1-Indanol, 2-(dodecylsulfinyl)- (6CI) (CA INDEX NAME)



L8 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:73337 CAPLUS
DOCUMENT NUMBER: 56:73337
ORIGINAL REFERENCE NO.: 56:14179h-i,14180a-i,14181a-b
TITLE: Organic sulfur compounds. VI. The effect of alkylamines on the course of the cooxidation of mercaptans and indene
AUTHOR(S): Oswald, Alexis A.; Noel, Fernand; Fisk, George
CORPORATE SOURCE: Imp. Oil Co., Sarnia, Can.
SOURCE: Journal of Organic Chemistry (1961), 26, 3974-80
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB In the presence of alkylamines, mercaptans, and indene (I) were cooxidized by mol. O with a chain mechanism to form substituted 2-mercapto-1-indanols, disulfides, and H2O, instead of substituted 2-mercapto-1-indanyl hydroperoxides. The initiation reaction forming the mercapto radicals could take place between alkylammonium thiolates and O. The change of the reaction products was due to the catalysis by the amines of the oxidation of mercaptans by substituted 2-mercapto-1-indanyl hydroperoxides. It was proposed that this catalytic action was important in the stabilization of some hydrocarbon fuels by alkylamines. In the cooxidn. expts., the O or air was introduced through a sintered glass inductor, mixture stirred, and the pressure kept slightly above atmospheric The reactions were followed by determining the decrease of the thiol concentration by potentiometric titration of samples with AgNO3. 2-(2-Naphthylthio)-1-indanyl hydroperoxide (II) (14.2 g.) in 2.5 l. PhMe, 6.6 g. benzenethiol (IIa), and 7.6 g. 1,1,3,3-tetramethylbutylamine (III) left 0.5 hrs., the solution evaporated in vacuo, at first 2-(2-naphthylsulfinyl)-1-indanol removed, then the solvent evaporated, and from the residue III and diphenyl disulfide removed by leaching with 2 60-ml. portions of heptane, and the product crystallized gave 5.2 g. 2-(2-naphthylthio)-1-indanol (IIIa), m. 141-3° (PhMe). IIa (13.2 g.) and 7.7 g. III in 250 ml. C6H6 treated with 19.4 g. 79% 2-phenylthio-1-indanyl hydroperoxide, the mixture stirred another hr. and evaporated, and the residue crystallized gave 5 g. 2-phenylthio-1-indanol (IIIb), m. 103-4° (heptane). A yield of 4.2 g. (PhS)2 was also obtained in this experiment II (6.3 g.) in 25 ml. Et2O added slowly to 1.1 g. triethylenediamine in 10 ml. Et2O (an exothermic reaction occurred) and

the solid collected gave 6.7 g. triethylenediammonium 2-(2-naphthylthio)-1-indanyl peroxide (IV), m. 89-90°. The synthesis of IV was also accomplished in PhMe. IIa (1.1 g.) in 80 ml. PhMe treated with 1.8 g. IV (slowly), the mixture left 0.5 hr. and filtered, and the solid recrystd. gave 1.2 g. IIIa. 2-Naphthalenethiol (6.4 g.) in 50 ml. PhMe treated 0.5 hr. at room temperature with 7.3 g. IV gave 8.8 g. addition product (V) of 2-(2-naphthylthio)-1-indanol and di-2-naphthyl disulfide, m. 126-7° (PhMe). IIIa (1.46 g.) and 1.6 g. di-2-naphthyl disulfide in 25 ml. PhMe heated, cooled to room temperature, and the crystals collected gave 2.5 g. V. A C6H6 solution (333 ml.) of 0.34 mole aromatic thiol, 0.11 mole I, and 0.01 mole of an alkylamine was oxygenated 6 hrs. at 22-8°. When benzenethiol and 2-naphthalenethiol were cooxidized with I in the presence of III, a yellow color developed. With 4-butylbenzenethiol, the mixture became dark yellow; with 4-toluenethiol and 4-chlorobenzenethiol, it became red and black, resp. When benzenethiol and I were cooxidized in the presence of mono-, di-, and tripropylamines, the formation of purple, green, and yellow colors were observed. After oxygenation, the C6H6 layer was decanted, the unchanged thiol removed from the C6H6 solution by washing with 5% KOH solution, the solvent distilled, and the residue fractionated to give 2-arylthio-1-indanols. The diaryl disulfides were too soluble in heptane and therefore were crystallized from MeOH. In the case of the 2-naphthalenethiol-I cooxidn., the reactant concns. were reduced to one-third, and C6H6 used as solvent of recrystn. because of the solubility of the addition compound of IIIa and di-2-naphthyl disulfide. The cooxidn. of IIa and I in the presence of III was also carried out on a 5 times larger scale in PhMe. After 6 hrs. of oxygenation, 58% of the thiol was oxidized and 4.4 g. of H2O separated By the extraction of the reaction mixture with 5% HCl and the concentration of the extract, 7 g. III.HCl was isolated. Workup of the PhMe solution gave 20.5 g. IIIb. A heptane solution (333 ml.) of 73.3 g. dodecanethiol, 22.9 g. I, and 4.2 g. III was oxygenated at 24-6° and the product, m. 69-72°, isolated. In addition to the above, the following substituted 2-mercapto-1-indanols were prepared (substituent, m.p., and % yield given): 4-tolyl, 95.5-6.5°, 64; 4-butylphenyl, 104-5°, 39; 4-chlorophenyl, 113.5-14.5°, 35.

2-Arylthio-1-indanol (0.01 mole) in AcOH was treated slowly at 50° with 1.1 g. 33% H2O2, the mixture kept 0.5 hr. at 60°, the resulting 2-arylsulfinyl-1-indanol precipitated by addition of H2O, the solid collected, and recrystd. from alc. Most of the oxidation products were identified with one isomer of the substituted 2-sulfinyl-1-indanols from the cooxidn. of I with the corresponding thiol in the absence of amine as shown (thiol starting material, m.p. of the 2-sulfinyl-1-indanol obtained by H2O2 oxidation given): benzene, 147-8.5° (decomposition); toluene, 144-5.5° (decomposition); 4-chlorobenzene, 146.5-8.0° (decomposition); 2-naphthalene, 134.5-6.0°; dodecane, 80-1°. An AcOH solution of 0.01 mole of 2-arylthio-1-indanol was oxidized with 2.3 g. 33% H2O2 as described above; the work up of the mixture (after being heated 1 hr. at 80°) yielded the 2-arylsulfonyl-1-indanols given below. The following substituted 2-sulfinyl-and 2-sulfonylindanols were thus obtained (R and x of RSOx, m.p., and % yield given): 4-butylphenyl, 1, 154-6°, 63; 4-dodecyl, 1, 80-1°, 71; 4-tolyl, 2, 145-6.5°, 72; 4-butylphenyl, 2, 156-8°, 98; 4-chlorophenyl, 2, 151.5-4.0°, 95; dodecyl, 2, 93.5-4.5°, 97. Benzene solns. containing 0.15 mole/l. of benzenethiol and 0.05 mole/l. I were oxygenated in the presence of various concns. of III at room temperature After 6 hrs. of oxygenation, the following decrease in % mercaptan was observed (amine mole/l., % thiol oxidized given): nil, 41; 0.015, 14; 0.150, 48; 0.300, 47. Primene 81-R was added to heptane solns. containing benzenethiol, I, and 2,5-dimethylpyrrole, the test solns. (300 ml. each) were aerated 6 hrs. at room temperature, and the following observations were made (mole/l. each of benzenethiol, I, and 2,5-dimethylpyrrole, mole/l. Primene 81-R, % thiol

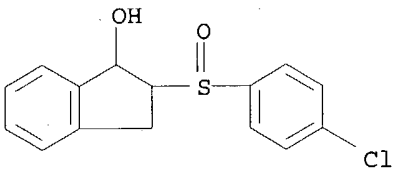
oxidized, peroxide formed, color of solution, and precipitate in g./100 ml. given):

0.30, nil, 68, yes, red, 3.5 (red oil); 0.30, 0.03, 56, no, colorless, 1.3 (colorless crystals); 0.01, nil, 75, yes, red, 0.2 (red solid); 0.01, 0.001, 53, no, colorless, none.

IT **62967-56-0**, 1-Indanol, 2-[(p-chlorophenyl)sulfinyl]- **92621-28-8**, 1-Indanol, 2-(phenylsulfinyl)- **93434-18-5**, 1-Indanol, 2-(p-tolylsulfinyl)- **94305-49-4**, 1-Indanol, 2-(2-naphthylsulfinyl)- **94385-24-7**, 1-Indanol, 2-[(p-butylphenyl)sulfinyl]- **102456-32-6**, 1-Indanol, 2-(dodecylsulfinyl)-
(preparation of)

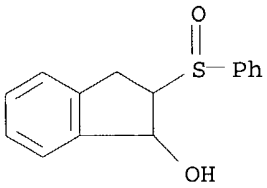
RN 62967-56-0 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



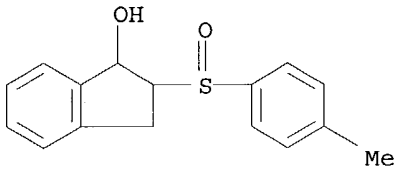
RN 92621-28-8 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



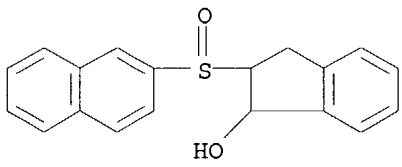
RN 93434-18-5 CAPLUS

CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)

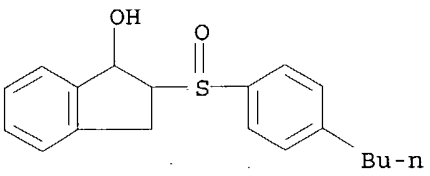


RN 94305-49-4 CAPLUS

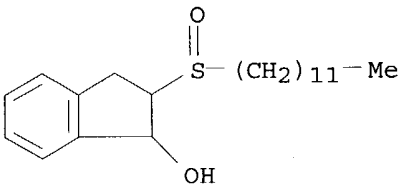
CN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



RN 94385-24-7 CAPLUS
CN 1-Indanol, 2-[(p-butylphenyl)sulfinyl]- (7CI) (CA INDEX NAME)



RN 102456-32-6 CAPLUS
CN 1-Indanol, 2-(dodecylsulfinyl)- (6CI) (CA INDEX NAME)



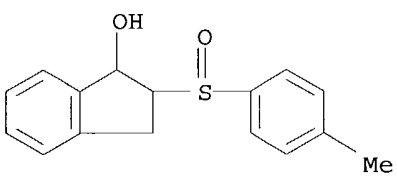
L8 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:47254 CAPLUS
DOCUMENT NUMBER: 56:47254
ORIGINAL REFERENCE NO.: 56:9005i,9006a
TITLE: Hydrocarbon purification process and catalyst
INVENTOR(S): Holden, Donald L.
PATENT ASSIGNEE(S): Universal Oil Products Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3016348		19620109	US	19591102

AB A catalyst is prepared by combining an Al2O3-SiO2 carrier material containing 10-25% SiO2 with 5-10% Mo and 1-5% Ni, then sulfiding so that the Mo and Ni exist as sulfides in the final composition Comparison of the liquid hydrogenation products obtained by use of this catalyst with those obtained by use of the well-known Al-Co-Mo catalyst showed marked improvement in the removal of N compds.

IT **93434-18-5**, 1-Indanol, 2-(p-tolylsulfinyl)-
(preparation of)

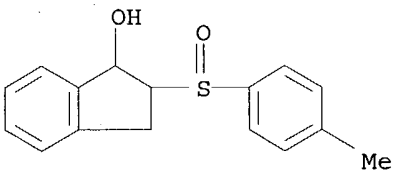
RN 93434-18-5 CAPLUS
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



L8 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:47253 CAPLUS
DOCUMENT NUMBER: 56:47253
ORIGINAL REFERENCE NO.: 56:9005h-i
TITLE: Denitrogenation of petroleum
INVENTOR(S): Oswald, Alexis A.; Rupar, Charles B.; Ilnyekyj, Stephen; Noel, Fernand
PATENT ASSIGNEE(S): Esso Research and Engineering Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3016349		19620109	US	19590810

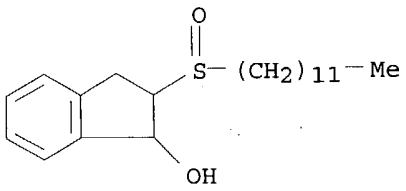
AB Addition of 0.5 to 3 moles of an organic peroxide such as Bz2O2, (4-ClC6H6)2O2, or tert-Bu2O2 per mole of pyrroles in the petroleum product at 50-250°F. converts the pyrrole-type compds. to higher-boiling compds. which are separated by distillation or filtration. Sulfides, such as 2-indanyl or p-tolyl sulfide, or sulfoxides, such as 2-phenyl-2-hydroxyethyl phenyl sulfoxide, may also be used, but at 60-360°F.
IT **93434-18-5**, 1-Indanol, 2-(p-tolylsulfinyl)-
(preparation of)
RN 93434-18-5 CAPLUS
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



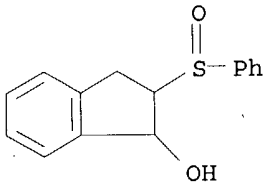
L8 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1961:124710 CAPLUS
DOCUMENT NUMBER: 55:124710
ORIGINAL REFERENCE NO.: 55:23460b-i,23461a-c
TITLE: Organic sulfur compounds. III. Cooxidation of mercaptans with styrenes and indene
AUTHOR(S): Oswald, Alexis A.
CORPORATE SOURCE: Imp. Oil Ltd., Sarnia, Can.
SOURCE: Journal of Organic Chemistry (1961), 26, 842-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 54, 21005e. PhSH (I) (0.1 mole) and 0.1 mole PhCH:CH2 (II) [or PhCMe:CH2 (III) or indene (IV)] in 310 ml. cold n-C7H16 bubbled through with air via a sintered glass sparger 6 hrs. at 0° yielded 30, 52, and 33% oily peroxides containing 84, 44, and 67% hydroperoxide, according to both the iodide and FeSO4 methods. Similar aeration of p-ClC6H4SH and III yielded 64% peroxide containing 58% hydroperoxide. A 4-g. sample of liquid substituted 2-mercaptoethyl hydroperoxide kept 3 days at 20° and the solid product recrystd. from PhMe-C7H16 yielded the corresponding isomeric 2-sulfinylethanol rearrangement products, RSO-CH2CR'PhOH (V). A typical member of these new hydroperoxides was 1-(2-naphthylthio)-2-phenyl-2-propyl hydroperoxide (VI), m. - 10°, peroxide content 85%, obtained by cooxidn. of 2-HSC10H7 and III. Phys. data were listed for V [R, R', m.p. (uncor.), and infrared OH, SO (2), aromatic and CH2

absorption peaks given]: Ph, H, 128-9.5°, 2.95, 9.23 (9.55), 10.02, 6.3, 6.9; 2-C10H7, H, 145-7° (121-6°), 3 (3.05), 9.5 (9.45), 9.9 (9.9), 6.28 (6.28), 6.91 (6.91); C12H25, H, 105-6° (69-70°), 3 (3), 9.3 (9.3), 9.85 (9.85), 6.25 (6.25), 6.9 (6.9); 4-ClC6H4, H, 156.5-8.5° (86-8°), 2.96 (2.96), 9.19 (9.19), 9.94 (9.96), 6.35 (6.35), 6.95 (6.95); 2-C10H7, Me, 115-18° (94-95.5°), 3.05 (3), 9.4 (9.4), 9.95 (9.78), 6.28 (6.28), 6.85 (6.93); C12H25, Me, 47.5-8.5°, 2.95, 9.4, 10.05, 6.25, 6.85. Similar rearrangements were carried out in 0.3M C6H6 (CHCl3, tetrahydronaphthalene) solns. of hydroperoxides at 43° in 16 hrs. VI (3.1 g.) yielded 27% V (R = 2-C10H7, R' = H), m. 115-18°, by this method. IV (11.6 g.) and 16 g. 2-C10H7SH in 100 ml. C6H6 and 300 ml. C7H16 aerated 4 hrs. at 0° yielded 4 g. crystalline 2-(2-naphthylthio)-1-indanyl hydroperoxide (VII), m. 70° (decomposition), containing 98% peroxide. The filtrate aerated 6 hrs. at 0° and 42 hrs. at 20°, filtered, and the cooxidn. product (26 g., containing only 2% peroxide) recrystd. from C6H6-C7H16 gave the 2-(2-naphthylsulfinyl)-2-indanoisomers, C6H4.CH(OH).CH(SOR).CH2 (VIII, R = 2-C10H7) (IX), m. 157-8°, m. 149-50°, m. 138.5-9.5° (decomposition), m. 125-7.5° (decomposition) (infrared spectrum given for all). VII (9.2 g.) in 100 ml. C6H6 kept 16 hrs. at 43° gave a neg. peroxide test and deposited 36.8 g. crystals, m. 138.5-9.5° (C6H6), identical with an isomer of IX. VII stored 10 min. in a desiccator at 2 mm. over H2SO4 decomposed violently and the reddish product fractionally crystallized from C6H6 gave IX, m. 157-8° and 138.5-9.5°. IV (10.7 g.) and 12.8 g. 4-ClC6H4SH in 250 ml. C6H6 and 20 ml. PhCl at 0° aerated 4 hrs. and the fresh peroxide solution refluxed 1 hr. in Et2O with LiAlH4 yielded 68% 2-(4-chlorophenylthio)-1-indanol (X), m. 110-12°. VII (6.0 g.) in 600 ml. C6H6, 150 ml. CHCl3, and 20 ml. MeOH kept 3 days at 20° with 4.3 g. X gave unchanged X and IX, m. 157-8°, suggesting an intramol. rearrangement. However, the reactions of the hydroperoxide cooxidn. intermediate might involve radical intermediates as was suggested by the polymerization of II by VII. VII (0.3 g.) in 34.6 g. II kept 3 months at 5° gave only 75% recovered II on distillation at 100°/20 mm., whereas II kept alone under the same conditions was distilled with 99% recovery. Aliphatic hydrocarbon (C7H16, cetane, straight run petroleum distillate, b. 70-200°) (300 ml.) containing 0.1 mole thiol, p-RC6H4SH (R = H, Me, 4-ClC6H4, and II, III, or IV aerated (or oxygenated) 3 days at 20° to give a liquid phase with peroxide number and mercaptan number less than 5 and 10, resp., the residue on filtration recrystd. from Ph-Me-C7H16 to give 40-80% mixts. of isomeric substituted 2-sulfinyl ethanols, and the mixts. recrystd. gave (with about 30% yield loss) the isomeric VIII (R and m.p. given) (infrared spectra given): Ph, 158-9°; 148-50°, 132-5°; p-MeC6H4, 166-7.5°, 144-4.5°, 128-30°; p-ClC6H4, 144-6°; C12H25, 107-9°, 67-8.5°. C12H25SH (20.2 g.) and 0.1 mole II (III, IV) in 300 ml. C7H16 aerated in a Vycor (95% quartz) flask with ultraviolet irradiation (GE-9T64Y20 lamp, 250 v., 1000 w. at 4.5 cm.) with decrease to less than 10% thiol content, the mixture cooled (solid CO2-alc. bath), and the product recryst. gave 75% VIII (R = C12H25) isomers. Cooxidn. of C12H25SH with III and IV gave only 10% V (R = C12H25, R' = Me) and 31% VIII (R = C12H25), m. 107-9°. Cetane (300 ml.) containing 0.01 mole/l. 2-C10H7SH and 0.01 mole II (IV) kept in a 500 ml. open pyrex flask showed rapid peroxidn. followed by a decrease in peroxide content, though the components in cetane showed no peroxidn. After 70 and 23 hrs. the IV-thiol and II-thiol solns. gave some IX, m. 138.5-9.5° (decomposition), and V (R = 2-C10H7, R' = H), m. 145-7°. Cetane (300 ml.) containing 0.3 mole/l. mercaptans and II or IV kept 2 weeks in accelerated storage tests at 43° and the ppts. recrystd. from C6H6-C7H16 gave the corresponding VIII. Distillation of the mother liquors yielded about 200 mg. 2-indanyl Ph sulfide and 180 mg. 2-indanyl 4-tolyl sulfide, resp. The reported reactions may be important in causing hydrocarbon fuel instability.

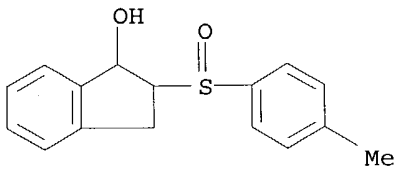
IT **102456-32-6**, 1-Indanol, 2-(dodecylsulfinyl)-
(isomer)
RN 102456-32-6 CAPLUS
CN 1-Indanol, 2-(dodecylsulfinyl)- (6CI) (CA INDEX NAME)



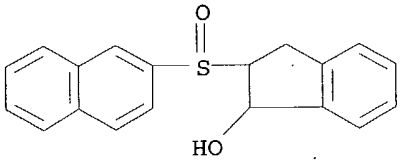
IT **92621-28-8**, 1-Indanol, 2-(phenylsulfinyl)- **93434-18-5**,
1-Indanol, 2-p-tolylsulfinyl- **94305-49-4**, 1-Indanol,
2-(2-naphthylsulfinyl)-
(isomers)
RN 92621-28-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



RN 93434-18-5 CAPLUS
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



RN 94305-49-4 CAPLUS
CN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)

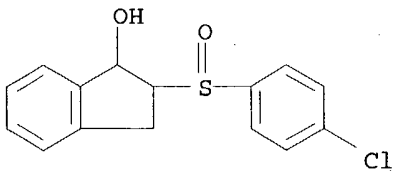


IT **62967-56-0**, 1-Indanol, 2-(p-chlorophenylsulfinyl)-
92621-28-8, 1-Indanol, 2-(phenylsulfinyl)- **93434-18-5**,
1-Indanol, 2-p-tolylsulfinyl- **94305-49-4**, 1-Indanol,
2-(2-naphthylsulfinyl)- **102456-32-6**, 1-Indanol,

2-(dodecylsulfinyl)-
(preparation of)

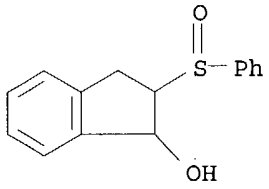
RN 62967-56-0 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



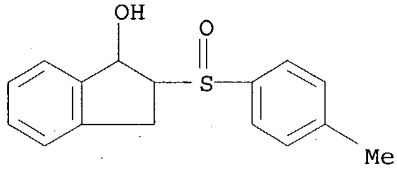
RN 92621-28-8 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



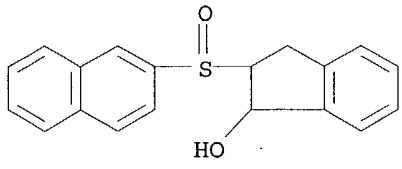
RN 93434-18-5 CAPLUS

CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



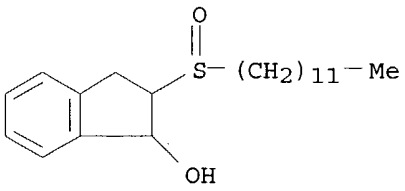
RN 94305-49-4 CAPLUS

CN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



RN 102456-32-6 CAPLUS

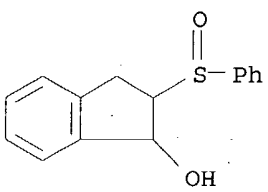
CN 1-Indanol, 2-(dodecylsulfinyl)- (6CI) (CA INDEX NAME)



L8 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1961:32998 CAPLUS
DOCUMENT NUMBER: 55:32998
ORIGINAL REFERENCE NO.: 55:6451b-e
TITLE: The cooxidation of olefins and mercaptans
AUTHOR(S): Ford, J. F.; Pitkethly, R. C.; Young, V. O.
CORPORATE SOURCE: Brit. Petrol. Co. Ltd., Middlesex, UK
SOURCE: Am. Chem. Soc., Div. Petrol. Chem., Preprints (1957), 2(No. 1), 111-22
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The primary and secondary products of the cooxidn. of indene (I) and thiophenol (II) were investigated. This was chosen as a simple synthetic system known to be related to the mixts. found in practice (gum-forming). Hydroperoxide was shown to be the main primary product, from which hydroxysulfoxides were formed by spontaneous rearrangement. These results were consistent with those of Kharasch. Results of a typical run at 20° were shown as a graph of O uptake and hydroperoxide and sulfoxide concns. vs. time. Initially almost all the O was used up to form the hydroperoxide (IIa), but concentration of this product fell with increasing sulfoxide concentration IIa was not isolated as such, but was reduced by LiAlH4 to trans-2-phenylmercapto-1-indanol (III). The combined reaction mixts. from 3 runs were maintained at 20° until decomposition of the peroxide was complete. From this mixture were isolated and identified by infrared spectrum and mixed m.p. with synthetic compds. (weight-% given): I, 3.7; trans-2-phenylsulfinyl-1-indanols (IVa), m. 150°, and IVb, m. 99°, total 79.1; III.1.9 and diphenyl disulfide, 1.7; in addition an oxosulfoxide fraction, 8.93 and 7 other fractions in small amts. were separated and characterized by infrared spectra. The following synthetic compds. were prepared for comparison with oxidation products: III and its cis-isomer; IVa and IVb and their cis-isomers of high and low m.p.; cis- and trans-2-phenylsulfonyl-1-indanol; trans-1-phenylmercapto-2-indanol; trans-1-phenylsulfinyl-2-indanols, m. 158° and 134°, resp.; trans-1-phenylsulfonyl-2-indanol, and some intermediates. The synthesis of these compds. was discussed.

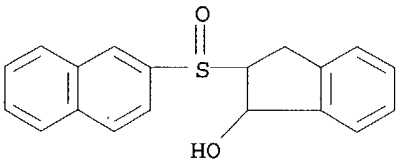
IT **92621-28-8**, 1-Indanol, 2-(phenylsulfinyl)- (stereoisomers)
RN 92621-28-8 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1960:50305 CAPLUS
DOCUMENT NUMBER: 54:50305
ORIGINAL REFERENCE NO.: 54:9855f-i
TITLE: Organic sulfur compounds. I. Hydroperoxide intermediates in the co-oxidation of mercaptans and olefins
AUTHOR(S): Oswald, Alexis A.
CORPORATE SOURCE: Imp. Oil Ltd., Sarnia, Can.
SOURCE: Journal of Organic Chemistry (1959), 24, 443-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Air introduced into mixts. of aromatic mercaptans (PhSH, p-MeC6H4SH, p-ClC6H4SH, β-C10H7SH) with reactive olefins (PhCH:CH2, PhCMe:CH2, indene) in hydrocarbons at 0° or lower temps. gave viscous intermediates of high hydroperoxide content. The new S-containing hydroperoxides, RSCHR1CR22OOH usually rearrange at room temperature to the corresponding hydroxyethyl sulfoxides, RSOCHR1CR22OH, with loss of peroxide content, increased absorption in the infrared at 3 and 9-10 μ and by solidification. Indene and β-C10H7SH gave an exceptionally stable co-oxidation product, 2-(2-naphthyl thio)-1-indanyl hydroperoxide, m. 70° (C6H6-C7H16), containing 98% peroxide, rearranging in C6H6 at 40° to give mainly 2-(2-naphthylsulfinyl)-1-indanol, m. 138.5-9.5° (decomposition). Co-oxidation of β-C10H7SH and PhCMe:CH2 gave 2-hydroperoxy-2-phenylpropyl 2-naphthyl sulfide, m. 10°, containing 85% peroxide, rearranged in C6H6 at 40° in 16 hrs. to give 2.3 g./100 ml. sediment, recrystd. (C6H6) to give 2-hydroxy-2-phenylpropyl 2-naphthyl sulfoxide, m. 114-18°. It was suggested that co-oxidation of mercaptans and olefins resulting in formation of hydroperoxides was largely responsible for peroxidation and subsequent color, gum, and sediment formation in untreated petroleum distillates.

IT **94305-49-4**, 1-Indanol, 2-(2-naphthylsulfinyl)-
(preparation of)
RN 94305-49-4 CAPLUS
CN 1-Indanol, 2-(2-naphthylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



L8 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1959:67657 CAPLUS
DOCUMENT NUMBER: 53:67657
ORIGINAL REFERENCE NO.: 53:12253b-i,12254a-i
TITLE: Stereochemistry of the cooxidation products of indene and thiophenol
AUTHOR(S): Ford, J. F.; Pitkethly, R. C.; Young, V. O.
CORPORATE SOURCE: British Petr. Co., Ltd., Sunbury-on-Thames, UK
SOURCE: Tetrahedron (1958), 4, 325-36
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The major primary product of the cooxidation of indene (I) and thiophenol (II) is trans-2-phenylthio-1-indanyl hydroperoxide (III), spontaneously rearranging to the two racemates of trans-2-phenylsulfinyl-1-indanol (IV,

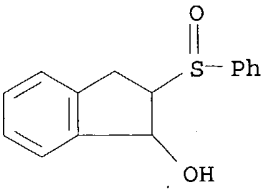
V). Attack by the PhS radical on I takes place, within 5%, exclusively at the 2 position and subsequent addition of O to the intermediate 2-phenylthioindanyl radical is, within the same limits, exclusively a trans addition The cis- and trans-2-phenylthio-1-indanols (VI, VII) and the related sulfoxides and sulfones were synthesized. Under certain conditions the substitution reaction of PhS ion with I bromohydrin is accompanied by migration of the HO group and production of trans-1-phenylthio-2-indanol (VIII). The sulfoxides and sulfones in this series were synthesized. Purification by distillation under N (O content not greater than 0.001%) gave 99.5% pure I, b13 67°, n20D 1.5765, f.p. - 1.549° and II, b13 69°, n20D 1.5899. I (0.046 mole) and 0.045 mole II in 150 ml. C6H6 shaken 85 min. at 20 ± 0.1°/760 ± 5 mm. with absorption of 0.043 mole O and the mixture [containing 7 and 77%, resp., of the absorbed O as sulfoxide and hydroperoxide according to the method of Barnard and Hargrave (C.A. 46, 7474i), with addition of 10 ml. AcOH to ensure solubility of the sulfoxides in the aqueous media] kept 140 hrs. at 20° gave a rise in sulfoxide concentration to 45% absorbed O and a complete decay of hydroperoxide according to a 2nd law reaction. The mixture at the end of the oxidation cooled rapidly to 5° and shaken with anhydrous MgSO4, the filtered solution added slowly to 4 g. LiAlH4 in 150 ml. tetrahydrofuran at 0° (hydroperoxide content half-way through the addition, 69% O uptake), the reduction mixture refluxed 6 hrs. and treated with water and aqueous NaOH, extracted with C6H6, and the product (9.05 g.) chromatographed on silica gel gave 7.19 g. VII (infrared absorption spectra were recorded for all substances described). Separate (3) cooxidations of 5.33 g. I and 4.95 g. II in 300 ml. C6H6 at 20° with 1.347 g. O were carried out, the combined products kept 140 hrs. at 20° to completion of decay of III and deposition of 8.0 g. crystals, m. 140-5°, the solution decanted, and the deposits recrystd. (C6H6) gave the high-melting isomer IV, m. 150°. The solution diluted with an equal volume of C5H12 and filtered yielded 8.3 g. mixture (of IV and V), m. 80-125°. The filtrate evaporated in vacuo and the residue distilled in a high vacuum to recover 1.3 g. I, the residue triturated with CCl4, and the crystalline product (8.3 g.) crystallized (C6H6-C6H12) gave the low-melting isomer V, m. 99°. The mother liquors evaporated, the viscous oil (8.76 g.) adsorbed on silica gel, and eluted by solvents of increasing polarity gave 0.6 g. Ph2S2, m. 61°, 0.65 g. VII, 1.50 g. IV, and 1.4 g. mixture of IV and V, accounting for 86% absorbed O. The remaining fractions consisted of unidentified sulfides, ketones, oxo sulfides and oxo sulfoxides, as indicated by infrared spectra. IV, V, and the mixture of IV and V oxidized in AcOH with a 5-fold excess of 30% H2O2 gave theoretical yields of trans-2-phenylsulfonyl-1-indanol (IX). A mixture of 95% IX (by weight) and 5% cis-2-phenylsulfonyl-1-indanol (X) began to liquefy at 105° and completely melted at 115°. The crude hydroxy sulfone obtained from the mixture (m. 80-125°) m. 115-17.5° and consequently the % content of cis isomers was less than 5%. I bromohydrin, m. 130° (prepared according to Pope and Read, C.A. 6, 3406), oxidized with CrO3-AcOH gave 61% 2-bromo-1-indanone, m. 33.5-4.5°. The bromo ketone (0.2 mole) in 200 ml. MeOH added slowly (N atmospheric) to NaSPh (from 5 g. Na and 0.196 mole II in 150 ml. dry MeOH), the mixture refluxed 15 min., 175 ml. MeOH distilled and the solution refluxed 1 hr., poured into 1 l. water and extracted repeatedly with C6H6, the washed (5% aqueous NaOH and water) and dried (anhydrous MgSO4) extract evaporated, and the residue recrystd. (C6H12) gave 48.4 g. product, m. 65-7.5°, recrystd. (C6H6-C6H12) to yield pure 2-phenylthio-1-indanone (XI), m. 66-7°; semicarbazone m. 188°; 2,4-dinitrophenylhydrazone m. 191°. XI (4.2 g.) in 30 ml. Et2O (dried over Na) added with stirring to 1 g. LiAlH4 in 50 ml. dry Et2O, the mixture refluxed 3 hrs., worked up according to Nystrom and Brown (C.A. 41, 4772g), and the product (4.08 g.) fractionally crystallized (C6H6-C6H12) yielded 64% VII, m. 102° (phenylurethan m. 121°), and 14% VI, m. 72°; phenylurethan m. 124°. Desulfurization of VII with Raney Ni gave

indan, n20D 1.5380, identified by its retention volume on a gas chromatography column. Attempted isomerization of VI by heating 4 hrs. with LiAlH4 in Et2O and by refluxing 4 hrs. (N atmospheric) with 10% alc. KOH gave only VI. VII (0.2 g.) refluxed 8 hrs., with 2 ml. 10% alc. KOH, the mixture neutralized with CO2, and the filtered and decolorized solution evaporated gave 0.12 g. material, m. 80-90°, containing 50% decomposition products other than VI. VII (0.5 g.) heated 4 hrs. in an evacuated sealed tube with 10% alc. KOH at 100° and the mixture worked up with CO2 gave only unchanged VII. VII (1.15 g.) in AcOH at 5° treated with 10% excess 30% H2O2, the mixture kept 24 hrs. at room temperature, and the 1.23 g. product fractionally crystallized (C6H6-C6H12) gave 0.31 g. IV, m. 149.5-50.5°, and 0.25 g. V, m. 99°. Desulfurization of VII with Raney Ni yielded indan. Similar oxidation of 2.6 g. VI and separation of the colorless gum (2.3 g.) gave the two cis-2-phenylsulfinyl-1-indanols (XII) and (XIII), m. 158°, and 122-3°, resp. The infrared spectra of XII and XIII were similar but differed considerably from those of IV and V. VII (0.75 g.) oxidized in CHCl3 by shaking with acid aqueous KMnO4 and working up according to Cunneen (C.A. 41, 3447a) yielded 0.3 g. IX, m. 122°. Oxidation of VI, XII, and XIII in AcOH with 5-fold excess of 30% H2O2 and crystallization of the products from C6H6-C6H12 yielded 95% X, m. 131°. Oxidation of VII, IX, and X (2 millimoles) at 40° in 20 min. with 4 millimoles CrO3 and KMnO4 oxidation of XI and VI yielded 2-phenylsulfonyl-1-indanone, m. 147-8°; 2,4-dinitrophenylhydrazone m. 262° (EtOAc). The reaction between trans-I bromohydrin (XIV) and NaSPh was found sensitive to reaction conditions and data on quantities of reactants and products formed are tabulated. In expts. 1 and 3, although the concns. were 50% higher in the latter, the proportions were identical (6% excess NaSPh and an addnl. 12% excess PhSH). It is probable that VII and VI were present in both products with the yield of VI appreciably higher in experiment 3 than in experiment 1. In experiment 2 the excess of NaSPh over XIV was only 1% but the mixture contained NaOEt derived from the 10% excess Na. The product was an oil containing small proportions of VI and VII but the major constituent yielded 2-indanol (XV) on desulfurization with Raney Ni and the reaction must have involved migration of the HO group with formation of VIII. Oxidation of the product (10 g.) in AcOH with 10% excess 30% H2O2, the oily product (10 g.) triturated with C6H6, and the solid (4.6 g., m. 145-8°) recrystd. (C6H6) yielded the high melting isomer of trans-1-phenylsulfinyl-2-indanol (XVI), m. 157-°. The mother liquors evaporated and the residue (4.0 g.) crystallized (1:1 C6H12-C6H6) gave the low melting isomer of trans-1-phenylsulfinyl-2-indanol (XVII), m. 133-4.5°. Desulfurization of 0.6 g. XVI in 80 ml. alc. with Raney Ni gave XV, m. 68-9°; phenylurethan m. 131-2°. The final mother liquors gave a solid (0.7 g.), recrystd. (C6H6-C6H12) to trans-1-phenylsulfonyl-2-indanol (XVIII), m. 113.5-14.5°. Oxidation of XVI and XVII in AcOH with excess 30% H2O2 gave theoretical yields of XVIII. I epoxide (0.35 mole prepared according to Boeseken and van Loon, C.A. 13, 314) treated according to Bordwell and Kern (C.A. 49, 9639g) with 0.36 mole NaSPh in 50% alc. gave 9.05 g. impure partially dehydrated VIII, n20D 1.6294; phenylurethan m. 146-7° (C6H12). By reducing the dielectric constant of the medium and increasing the PhS- concentration the SN1 mechanism was inhibited and the SN2 promoted. Experiment 4 was carried out with a 4-fold excess of PhS- and PhSH containing a min. amount of alc. was used as solvent. The 89% yield was virtually pure VI, providing convincing confirmation of the assignments of configuration made on the evidence of yields of isomers from the LiAlH4 reduction of XI, namely that VII, m. 102°, is trans and VI, m. 72°, is cis.

IT **92621-28-8**, 1-Indanol, 2-(phenylsulfinyl)- (stereoisomers)

RN 92621-28-8 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	105.52	271.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-15.25	-15.25

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